

The Calibration problem

Stat 524
10-26-17

In Simple linear regression,

①

you are given a particular y^*

and asked to estimate the corresponding x^* .

Also, find a confidence interval.

True model is $y = \beta_0 + \beta_1 x + \epsilon$

Prediction equation is $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$

Given a y^* , solve the prediction equation ②

for x to get $\hat{x}^* = \frac{y^* - \hat{\beta}_0}{\hat{\beta}_1}$

Note: this involves the ratio of 2 estimators.

The Delta Method is a Taylor series method used to estimate expectations & variances of functions of estimators.

$$\text{Review: } f(u, v) \approx f(u_0, v_0) + \left. \frac{\partial f}{\partial u} \right|_{(u_0, v_0)} (u - u_0) + \left. \frac{\partial f}{\partial v} \right|_{(u_0, v_0)} (v - v_0) \quad (3)$$

$$f(u, v) = \frac{c-u}{v} \approx \frac{c-u_0}{v_0} + \left(-\frac{1}{v_0}\right)(u-u_0) + \left(-\frac{c-u_0}{v_0^2}\right)(v-v_0)$$

$$\frac{\partial f}{\partial u} = -\frac{1}{v}, \quad \frac{\partial f}{\partial v} = (c-u) \frac{-1}{v^2}$$

$$\text{Choose } u_0 = \beta_0 \text{ and } v_0 = \beta_1 \quad (4)$$

Then

$$\hat{x}^* = \frac{y^* - \hat{\beta}_0}{\hat{\beta}_1} \approx \frac{y^* - \beta_0}{\beta_1} - \frac{1}{\beta_1} (\hat{\beta}_0 - \beta_0) - \frac{(y^* - \beta_0)}{\beta_1^2} (\hat{\beta}_1 - \beta_1)$$

$$\text{So } E[\hat{x}^*] \approx \frac{y^* - \beta_0}{\beta_1} - 0 - 0 = x^*$$

$\therefore \hat{x}^*$ is approximately unbiased

$$\begin{aligned}
 V[\hat{x}^*] &\approx \frac{1}{\beta_1^2} V[\hat{\beta}_0] + \frac{(y^* - \beta_0)^2}{\beta_1^4} V[\hat{\beta}_1] \quad (5) \\
 &\quad + \frac{2(y^* - \beta_0)}{\beta_1^3} \text{Cov}[\hat{\beta}_0, \hat{\beta}_1] \\
 &= \frac{1}{\beta_1^2} \left[V[\hat{\beta}_0] + \left(\frac{y^* - \beta_0}{\beta_1} \right)^2 V[\hat{\beta}_1] \right. \\
 &\quad \left. + 2 \frac{y^* - \beta_0}{\beta_1} \text{Cov}[\hat{\beta}_0, \hat{\beta}_1] \right]
 \end{aligned}$$

$$\begin{aligned}
 V[\hat{x}^*] &\approx \frac{1}{\beta_1^2} \left[V[\hat{\beta}_0] + (x^*)^2 V[\hat{\beta}_1] + 2x^* \text{Cov}[\hat{\beta}_0, \hat{\beta}_1] \right] \quad (6) \\
 &= \frac{1}{\beta_1^2} V[\hat{\beta}_0 + x^* \hat{\beta}_1] \\
 &= \frac{1}{\beta_1^2} \sigma^2 \left[1 + \frac{1}{n} + \frac{(x^* - \bar{x})^2}{S_{xx}} \right] \quad \left(\begin{array}{l} \text{variance of} \\ \text{a single new} \\ \text{predicted} \\ \text{y-value} \end{array} \right)
 \end{aligned}$$

$$\hat{V}[\hat{x}^*] = \frac{1}{\hat{\beta}_1^2} \hat{\sigma}^2 \left[1 + \frac{1}{n} + \frac{(\hat{x}^* - \bar{x})^2}{S_{xx}} \right]$$

(6)

$$\begin{aligned}
 V(\hat{x}^*) &\approx \frac{1}{\beta_1^2} \left[V(\hat{\beta}_0) + (x^*)^2 V(\hat{\beta}_1) + 2x^* \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) \right] \\
 &= \frac{1}{\beta_1^2} V[\hat{\beta}_0 + x^* \hat{\beta}_1] \\
 &= \frac{1}{\beta_1^2} \sigma^2 \left[1 + \frac{1}{n} + \frac{(x^* - \bar{x})^2}{S_{xx}} \right] \quad \left(\begin{array}{l} \text{variance of} \\ \text{a single new} \\ \text{predicted} \\ \text{y-value} \end{array} \right)
 \end{aligned}$$

$$\hat{V}(\hat{x}^*) = \frac{1}{\hat{\beta}_1^2} \hat{\sigma}^2 \left[1 + \frac{1}{n} + \frac{(\hat{x}^* - \bar{x})^2}{\hat{S}_{xx}} \right]$$

(8)

$$\ln y = \ln \beta + \alpha x$$

Suppose we fit $\ln y = \beta_0 + \beta_1 x + \varepsilon$

Then $e^{\ln y} = e^{\beta_0 + \beta_1 x + \varepsilon}$

$$y = e^{\beta_0} e^{\beta_1 x} e^{\varepsilon}$$

Note that the error term is now
multiply instead of additive

Some other linearizing transformations

(9)

are the logit, to linearize an "S" shape

• Gompertz for a variety of shapes

$$\ln y = \beta_0 + \beta_1 \ln x + \varepsilon$$

$$y = e^{\beta_0} e^{\beta_1 \ln x} e^{\varepsilon} = e^{\beta_0} x^{\beta_1} e^{\varepsilon} \quad \text{power model}$$

Normalizing transformations

(10)

Goal: find a transformation of Y ,

so that the resulting residuals
will be normally distributed.

Box-Cox transformation: $W = \frac{Y^\lambda - 1}{\lambda}$

$$\lim_{\lambda \rightarrow 0} \frac{Y^\lambda - 1}{\lambda} = \lim_{\lambda \rightarrow 0} \frac{Y^\lambda \ln Y}{1} = \ln Y$$

How did they find the best λ ?

(11)

$$\text{Let } w_i = \frac{y_i^\lambda - 1}{\lambda} \text{ for } i=1, \dots, n$$

Use the Jacobian method to find the relationship between the joint pdf of (w_1, \dots, w_n) and the joint pdf of (y_1, \dots, y_n)

$$f(y_1, \dots, y_n) = g(w_1, \dots, w_n) |J|,$$

where $J = \left[\frac{\partial w_i}{\partial y_j} \right]_{n \times n}$ i, j^{th} term

$$\text{For } i \neq j, \frac{\partial w_i}{\partial y_j} = 0$$

(12)

$$\text{For } i=j, \frac{\partial w_i}{\partial y_i} = \frac{1}{\lambda} \lambda y_i^{\lambda-1} = y_i^{\lambda-1}$$

$$J = \begin{bmatrix} y_1^{\lambda-1} & 0 & \dots & 0 \\ 0 & y_2^{\lambda-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & y_n^{\lambda-1} \end{bmatrix}$$

$$|J| = \left(\prod_{i=1}^n y_i \right)^{\lambda-1}$$

$$So \ f(y_1, \dots, y_n) = \underbrace{g(w_1, \dots, w_n)}_{\substack{\text{force this to} \\ \text{be the multivariate} \\ \text{normal pdf}}} (\prod y_i)^{\lambda-1} \quad (13)$$

$$f(y_1, \dots, y_n) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n e^{-\frac{1}{2\sigma^2} \sum (w_i - E(w_i))^2} \cdot (\prod y_i)^{\lambda-1}$$

Use maximum likelihood to find
the value of λ that maximizes this

There is no analytic solution, but $\hat{\lambda}$ can
be found numerically

In practice, choose λ close to the optimal $\hat{\lambda}$,
but easier to interpret

| | |
|-------------------------|---------------|
| $\lambda = \frac{1}{2}$ | \sqrt{y} |
| $\lambda = 2$ | y^2 |
| $\lambda = 0$ | $\ln y$ |
| $\lambda = -1$ | $\frac{1}{y}$ |

- 4.13** Problem 3.8 asked you to fit two different models to the chemical process data in Table B.5. Perform appropriate residual analyses for both models. Discuss the results of these analyses. Calculate the PRESS statistic for both models. Do the residual plots and PRESS provide any insight regarding the best choice of model for the data?
- 4.15** In Problem 3.9, you were asked to fit a model to the tube-flow reactor data in Table B.6.
- a.** Construct a normal probability plot of the residuals. Does there seem to be any problem with the normality assumption?
 - b.** Construct and interpret a plot of the residuals versus the predicted response.
 - c.** Construct the partial regression plots for this model. Does it seem that some variables currently in the model are not necessary?